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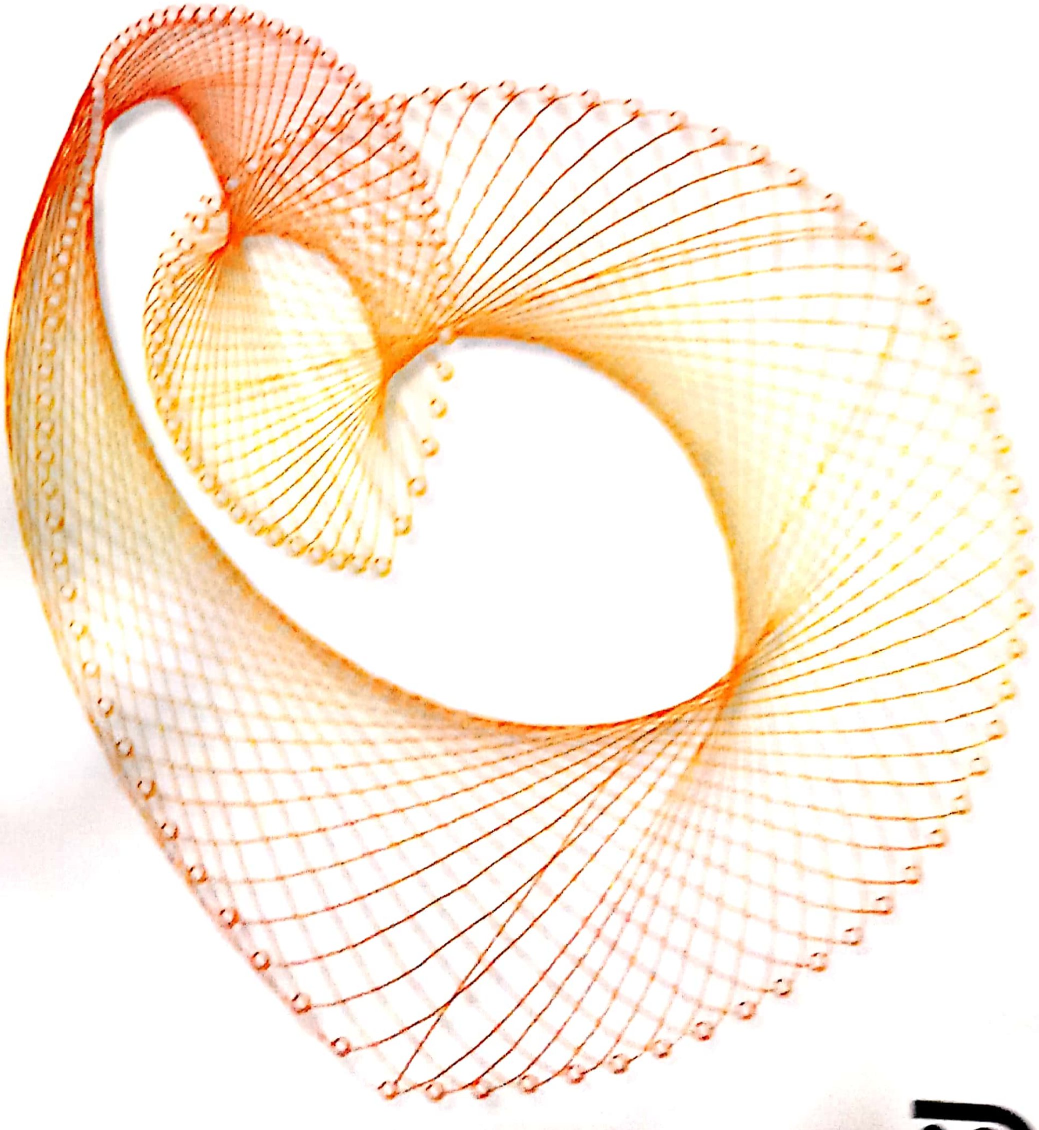

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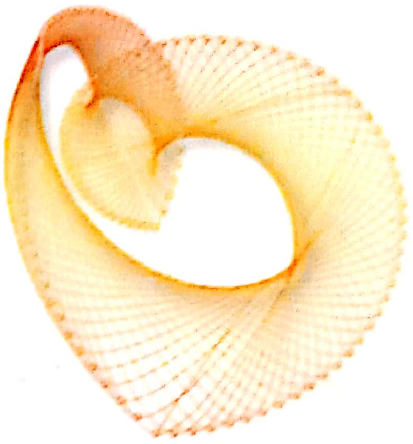
Group Theory
and its Applications

P. K. Patra • R. K. Thapa



GROUP THEORY AND ITS APPLICATIONS explains in detail how to determine the symmetry operations and symmetry elements of different molecules and then goes on to present how to determine the character tables of different groups with examples illustrating the procedure in full detail. Group theory is an abstract mathematical tool that underlies the study of symmetry and invariance. By using the concepts of symmetry and group theory, it is possible to obtain the members of complete set of known basis functions of the various irreducible representations of the group. In practice this is achieved by applying the projection operators to the linear combination of atomic orbitals (LCAO) when the valence electrons are tightly bound to the ions, to orthogonalized plane waves (OPW) when valence electrons are nearly free and to the other given functions that are [illegible]le to a particular system under consideration. In solid state physics, the [illegible]up theory is indispensable in the context of finding the energy bands of electrons in solids. It can also be applied to electron emission spectroscopy to derive basis functions by projection operator method to calculate currents like in photoemissions or photofield emissions. Group theory has many applications in physics and chemistry, for example, this is used to classify crystal structures, the symmetry of molecules and to determine physical properties such as polarity, spectroscopic properties useful for Raman spectroscopy and infrared spectroscopy and to construct molecular orbitals.

It is written for physicists at an introductory level, keeping in view that a beginner will be able to understand the concepts relevant to the treatment of problems in physics.

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Preface

Group theory is such a subject that it has become indispensable to anyone doing research works in Physics, Chemistry and Material Science. For example, if one would like to understand the dispersions of electrons, without understanding the symmetry, it will be difficult to study. One therefore needs first of all to find in which point group the electron belongs, what will be the appropriate point group operation and hence the symmetry direction or symmetry points. These will all lead to specific type of representation. To understand all these, it is better to first get the first hand knowledge about the basics of group theory.

This book on group theory with its application is written with the basic intention that it will meet the requirement of the post graduate students in Physics and Chemistry in Indian Universities. The authors have tried best to give the subject a very lucid treatment so that even at the first reading, the students will be able to grasp the concept easily. However, errors are going to be there for which the authors welcome the suggestions from its readers for its further improvement.

The authors would like to thank Prof. Sydney George Davison for sending the book Basic Theory of Surface States (1992) which in fact has given clarity in respect to many fundamental concepts of group theoretical topics. Dr. Sandeep, Dr. Dibya Prakash Rai, Dipendra Pradhan and Anup Shakya Pradhan have all helped in typing the manuscript to its present form. Dr. Amit Shankar and Dr. Sandeep has infact taken the troubles to correctly redraw all the figures to its final form.

Mrs. Prue Davison has been always showering the words of encouragement especially to Prof. Ram Kumar Thapa. She has also helped with enormous number of research papers due to which application of group theory was made possible in the case of two Ph.D. students who have worked on Photoemission and Photofield emission theories.

Authors are grateful to NAROSA PUBLISHING HOUSE, New Delhi, for their keen interest in the publication of the book at the earliest.

P. K. Patra
R. K. Thapa

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